

Wave-packet analysis of electron-phonon interaction in the Wigner formalism

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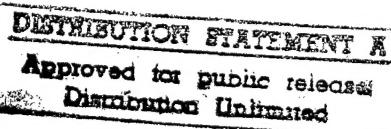
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Abstract

A theoretical and computational analysis is presented of the motion of a single one-dimensional electron, represented by a wave packet of given average momentum and position, in a fixed potential profile in presence of electron-phonon interaction. The electron propagation can take place with or without an external bias. A perturbative approach is used in the theoretical framework of the Wigner function accounting for the continuous quantum dynamical evolution of the scattering process. The unperturbed hamiltonian contains the one-dimensional potential profile and the external field, while the electron-phonon coupling potential is considered as the perturbation hamiltonian. Computational results are presented for the case of an electron propagating a) without applied forces, b) through a region where a uniform electric field is applied, and c) in a double-barrier potential in resonance conditions, due to the relevance of these physical cases for practical applications.



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I. INTRODUCTION

The quantum theory of electron transport has been extensively studied in the last decade in connection with the experimental development of mesoscopic structures and the engineering of low-dimensional electronic devices (see, e.g., [1–3]). In fact it appears that the length of the active region of many submicron structures is short enough to be of the order of the inelastic mean-free path (i.e., the distance over which carriers maintain phase information). Thus it is expected that quantum effects must appear in such devices.

Scattering destroys the phase coherence of the electron wave function and thus many relevant quantum effects. In most cases the scattering agents are acoustic and optical phonons. The efficiency of these mechanisms is related to the crystal temperature, but they can be present even at very low temperatures since acoustic phonons allow, in principle, exchange of arbitrary small energies.

Coherent transport, i.e. carrier transport in absence of phase-breaking scattering processes, has been widely treated in the literature through many possible theoretical approaches. Some attempts at including phonon scattering into the quantum theory have been presented in the literature, mainly based on simplified approaches where a relaxation-time approximation is used [4,5] or where the scattering is treated in the semiclassical approximation and the Wigner function is used as a classical distribution function [6] which, however, heavily deteriorates the quality of the rigorous quantum approach.

In the present paper a quantum theory of electron transport in semiconductors including coherent propagation and phonon interaction is presented in the framework of the Wigner approach. The use of the Wigner function (WF) has been found particularly appropriate for the theoretical analysis of quantum problems since it combines the rigorous quantum mechanical approach with the more familiar representation of phase space.

An equation is obtained for such a function by using an interaction picture where the electron potential profile, including the external bias, besides the free-phonon term, is incorporated in the unperturbed Hamiltonian. The equation is then expanded iteratively, and

the corresponding terms will contain one, two, ... n phonon interaction processes as it happens in the semiclassical case. In the present approach the continuum quantum dynamical evolution of the electron system during the phonon interaction can be followed.

A numerical technique has been developed which, at present, evaluates terms in the expansion of the WF up to the second order in the interaction hamiltonian, but in principle it can be extended to higher orders.

Section II illustrates the theoretical approach, while in Section III the numerical procedure used in the present paper is described in details. Results are shown in Section IV for a single electron wave packet moving a) in absence of external forces, b) in presence of a uniform electric field, and c) in a resonant tunnelling structure in resonance conditions. The physical situation of a single phonon emission during the propagation is considered in the three cases above. Some conclusions and perspectives are reported in Section V.

II. THEORETICAL APPROACH

A three-dimensional system of independent electrons interacting with phonons is considered here with translational invariance along two directions (x-y). The unperturbed hamiltonian H_o of the system contains the electron hamiltonian (including the potential profile $V(z)$), and the free-phonon term:

$$H_o = \frac{p^2}{2m} + V(z) + \sum_q a_q^\dagger a_q \hbar \omega_q \quad (1)$$

where p and m are the electron quasi-momentum and effective mass, respectively. For simplicity m is assumed constant along the device. $V(z)$ is the electron potential profile (including the applied voltage), a_q and a_q^\dagger are the annihilation and creation operators of the phonon mode q with frequency ω_q . The electron-phonon interaction is described by the Hamiltonian:

$$H_{ep} = \sum_q i\hbar F(q) [a_q e^{iqr} - a_q^\dagger e^{-iqr}] \quad (2)$$

where $F(q)$ is a function that depends on the considered type of electron-phonon interaction.

In our case polar optical phonons have been considered [7].

Three characteristic space regions are of interest for this problem. The potential is supposed to vary only inside the "P" region; the WF is evaluated on a larger "D" region which defines the device of interest; finally the system is supposed to be enclosed in a larger universe "U" region, so that at the boundaries of U all wave functions are supposed to vanish and in order to evaluate the WF only correlations within this region must be considered.

The present theoretical approach [8] starts from the definition of the WF, generalized to include a single electron (or, equivalently, many independent electrons) and phonons into the physical system of interest:

$$f_w(\mathbf{r}, \mathbf{p}; n_q, n'_q) = \frac{1}{h^3} \int d\mathbf{r}' e^{-i\frac{\mathbf{p}}{h}\mathbf{r}'} \rho(\mathbf{r} + \frac{\mathbf{r}'}{2}, n_q; \mathbf{r} - \frac{\mathbf{r}'}{2}, n'_q) \quad (3)$$

where ρ is the density matrix of the electron-phonon system.

For any given basis $\{|\phi_l\rangle\}$ for the electron states, it is possible to move from the WF to the density-matrix representation and viceversa by means of the following coefficients [9]:

$$f_{lm}(\mathbf{r}, \mathbf{p}) = \frac{1}{h^3} \int d\mathbf{r}' e^{-i\frac{\mathbf{p}}{h}\mathbf{r}'} \langle \mathbf{r} + \frac{\mathbf{r}'}{2} | \phi_l \rangle \langle \phi_m | \mathbf{r} - \frac{\mathbf{r}'}{2} \rangle \quad (4)$$

according to the following equations:

$$f_w(\mathbf{r}, \mathbf{p}; n_q, n'_q; t) = \sum_{n, n'} f_{n, n'}(\mathbf{r}, \mathbf{p}) \rho(n, n_q; n', n'_q; t) \quad (5)$$

$$\rho(n, n_q; n', n'_q; t) = h^3 \int d\mathbf{p} \int d\mathbf{r} f_{nn'}^*(\mathbf{r}, \mathbf{p}) f_w(\mathbf{r}, \mathbf{p}; n_q, n'_q; t) \quad (6)$$

where $\rho(n, n_q; n', n'_q; t)$ is the density matrix in the basis $\{|\phi_l\rangle\}$

Starting from the density-matrix operator in the interaction picture with \mathbf{H}_0 in Eq.1 as unperturbed hamiltonian, we can construct the associated WF \tilde{f}_w , which satisfies the following equation of motion:

$$\frac{\partial}{\partial t} \tilde{f}_w(\mathbf{r}, \mathbf{p}; n_q, n'_q; t) = \frac{1}{h^3} \int d\mathbf{r}' e^{-i\frac{\mathbf{p}}{h}\mathbf{r}'} \langle \mathbf{r} + \frac{\mathbf{r}'}{2}, n_q | [\tilde{\mathcal{H}}'(t), \tilde{\rho}] | \mathbf{r} - \frac{\mathbf{r}'}{2}, n'_q \rangle \quad (7)$$

where $\tilde{\mathcal{H}}'(t) = \frac{\hat{H}_{ep}}{i\hbar}$ is the normalized interaction Hamiltonian in the interaction picture.

After formal integration we obtain:

$$\begin{aligned} \tilde{f}_w(\mathbf{r}, \mathbf{p}; n_q, n_{q'}; t) = & \\ & \tilde{f}_w(\mathbf{r}, \mathbf{p}; n_q, n_{q'}; 0) + \int_0^t dt' \sum_{nn'} f_{nn'}(\mathbf{r}, \mathbf{p}) \\ & \sum_m \sum_{m_q} h^3 \int d\mathbf{r}' \int d\mathbf{p}' \{ \tilde{\mathcal{H}}'(n, n_q; m, m_q; t') f_{m,n'}^*(\mathbf{r}', \mathbf{p}') \tilde{f}_w(\mathbf{r}', \mathbf{p}'; m_q, n_{q'}; t') - \\ & f_{n,m}^*(\mathbf{r}', \mathbf{p}') \tilde{f}_w(\mathbf{r}', \mathbf{p}'; n_q, m'_q; t') \tilde{\mathcal{H}}'(m, m_q; n', n_{q'}; t') \} \end{aligned} \quad (8)$$

The same equation can be transformed into the Schrödinger picture as follows; using the coefficients in Eq.4 we obtain the density matrix in the interaction picture; then we transform this quantity to the Schrödinger picture, and return to the WF by means of the same coefficients. We finally obtain the following expression:

$$\begin{aligned} f_w(\mathbf{r}, \mathbf{p}; n_q, n'_{q'}; t) = & h^3 \sum_{nn'} f_{nn'}(\mathbf{r}, \mathbf{p}) e^{-i(\omega_{n,n_q} - \omega_{n',n'_{q'}})t} \\ & \int d\mathbf{r}' d\mathbf{p}' f_{nn'}^*(\mathbf{r}', \mathbf{p}') \tilde{f}_w(\mathbf{r}', \mathbf{p}'; n_q, n'_{q'}; t) \end{aligned} \quad (9)$$

Eq. 8 can be substituted into itself to obtain the Neumann series for our problem.

When electronic properties are searched for, a trace over the phonon variables must be performed, so that we are here interested in diagonal matrix elements in the phonon coordinates at time t . Furthermore, since we are interested in studying a single electron-phonon scattering process, we assume that at the initial time $t = 0$ electrons and phonons are not interacting, and the phonons are in the diagonal equilibrium state. This initial physical condition is close to the semiclassical description of a scattering event.

The zero-order term in the perturbation Hamiltonian yields the ballistic evolution of the WF:

$$\begin{aligned} f_w^{(0)}(\mathbf{r}, \mathbf{p}; n_q, n_q; t) = & h^3 \sum_{nn'} f_{nn'}(\mathbf{r}, \mathbf{p}) e^{-i\{\omega(n, n_q) - \omega(n', n_q)\}t} \\ & \int d\mathbf{r}' \int d\mathbf{p}' f_{nn'}^*(\mathbf{r}', \mathbf{p}') f_w(\mathbf{r}', \mathbf{p}', n_q, n_q; 0) \end{aligned} \quad (10)$$

The first-order correction contains a single matrix element of the electron-phonon interaction

hamiltonian. Under the hypothesis of initial and final diagonal phonon states the first-order corrections do not contribute to our analysis.

The second-order terms contain two matrix elements of the perturbation hamiltonian and can provide diagonal contributions at time t starting from diagonal contributions at $t = 0$, corresponding to a single phonon scattering. The quantum process can then be a “virtual” process if the coordinates of the phonon bath are the same in the initial and final states, or it can be a “real” process if the final phonon state contains one phonon more/less than the initial state. It is well known that virtual processes contribute to the self energy associated to the quantum state and reduce to the “out-scattering” term of the Boltzmann equation in the semiclassical limit, while real processes contribute to the “in-scattering” term.

As an example, the second-order correction associated to real-emission processes considered in the numerical calculations presented in this paper is given by:

$$\begin{aligned} \Delta f_w^{(2,r,E)}(\mathbf{r}, \mathbf{p}, t) = & \\ 2\Re \sum_{\mathbf{q}} F^2(\mathbf{q}) < n_q + 1 > \sum_{ll'} f_{ll'}(\mathbf{r}, \mathbf{p}) \sum_{ms} \mathcal{C}^*(m, q, l) \mathcal{C}(s, q, l') \\ \mathcal{T}^{(r,E)}(l, l', s, m; q; t) h^3 \int d\mathbf{r}' d\mathbf{p}' f_{ms}^*(\mathbf{r}', \mathbf{p}') f_w(\mathbf{r}', \mathbf{p}', 0) \end{aligned} \quad (11)$$

In the above equation $\mathcal{T}^{(r,E)}(l, l', s, m; q; t)$ contains the time-dependence of the considered perturbative correction:

$$\begin{aligned} \mathcal{T}^{(r,E)}(l, l', s, m; q; t) = & \\ \frac{e^{-i(\omega_l - \omega_{l'})t} - e^{-i(\omega_m - \omega_s)t}}{(\omega_{l'} - \omega_s + \omega_q)(\omega_m - \omega_l + \omega_{l'} - \omega_s)} + & \\ \frac{e^{-i(\omega_m - \omega_{l'} - \omega_q)t} - e^{-i(\omega_l - \omega_{l'})t}}{(\omega_{l'} - \omega_s + \omega_q)(\omega_m - \omega_l - \omega_q)} \end{aligned} \quad (12)$$

$\hbar\omega_n$ is the energy associated to the electron state $|\phi_n\rangle$ and $\mathcal{C}(m, q, l)$ is the matrix element of e^{iqr} between the electron eigenstates $|\phi_m\rangle$ and $|\phi_l\rangle$.

Eq. 12 is of the same nature of the time-dependent coefficient involved in the derivation of the Fermi Golden Rule. In that case however the transition induced by the perturbation

is considered between two eigenstates of the unperturbed Hamiltonian, while in the present case the "transition" occurs between two matrix elements of the density operator.

III. COMPUTATIONAL APPROACH

The perturbative corrections contained in the Neumann series obtained above can be evaluated with a suitable numerical technique, provided that the unperturbed electron eigenvalues and eigenvectors are known. However formidable numerical difficulties related to interference of quantum oscillations allow to evaluate, at present, terms up to the second-order, corresponding to a single scattering process.

A numerical solution of the time-independent Schrödinger equation for the unperturbed hamiltonian is here obtained for any given one-dimensional potential profile, including the heterostructure profile due to band discontinuity and, possibly, to an applied potential.

The state of the "sampling" electron is chosen at the initial time $t = 0$ in such a way to have a gaussian probability distribution in position and momentum space (minimum-uncertainty wave packet). The initial state is then propagated according to the time evolution associated to the unperturbed hamiltonian and the corresponding WF is evaluated accordingly. At time t_s we assume that the electron-phonon interaction is switched on. The second-order perturbative correction to the WF is then evaluated for a real single-phonon process at the observation time t .

Since only the second-order correction is evaluated from the numerical procedure, a time decaying factor $e^{-\Gamma(t-t_s)}$ has been associated to the unperturbed state for $t > t_s$ to account for the fact that, as time evolves from the initial condition, the scattering-out virtual processes decrease the unperturbed WF. Correspondingly the time-dependence of the second-order correction in Eq. 12 is modified as follows:

$$\begin{aligned} \mathcal{T}_\Gamma^{(r,E)}(l, l', s, m; q; t) = \\ \frac{\omega_{l'} - \omega_s + \omega_q + i\Gamma}{(\omega_{l'} - \omega_s + \omega_q)^2 + \Gamma^2} \left\{ \frac{e^{-i(\omega_m - \omega_s - 2i\Gamma)t} - e^{-i(\omega_l - \omega_{l'})t}}{(\omega_s - \omega_m + \omega_l - \omega_{l'} + 2i\Gamma)} + \right. \end{aligned}$$

$$\frac{\omega_m - \omega_l - \omega_q + i\Gamma}{(\omega_m - \omega_l - \omega_q)^2 + \Gamma^2} (e^{-i(\omega_m - \omega_{l'} - \omega_q - i\Gamma)t} - e^{-i(\omega_l - \omega_{l'})t}) \quad (13)$$

IV. RESULTS

Three cases of single-electron propagation are presented in this paper as important examples of application of the present theoretical approach. When a potential profile is present the eigenstates and eigenvalues of the system have been determined through a numerical solution of the associated Schrödinger equation.

In all cases the length of the U region is 10^4 Å , which allows to deal with normalized electron states, but it is large enough to not influence the electron dynamics under investigation. An effective mass $0.067m_e$ has been used and the electron initial gaussian wave packet is centered around the energy $0.03eV$, which corresponds to a resonant state of the quantum well between the two barriers discussed in Section IV C. As it regards the dynamical situation, a scattering process has been studied where, in semiclassical terms, the initial positive electron wave vector ($k_i = 0.23 \times 10^9 \text{ m}^{-1}$) is almost reversed by a phonon emission ($k_f = -0.20 \times 10^9 \text{ m}^{-1}$). The phonon equivalent temperature and wave vector have been chosen as $T = 100K$ and $q = 0.43 \times 10^9 \text{ m}^{-1}$. The unperturbed WF has been exponentially damped with time through a damping factor $\Gamma^{-1} = 1.5 \text{ ps}$.

The amplitude of the second-order correction of the WF (scattered electron) will be shown artificially amplified for graphic reasons. This correction is always many orders of magnitude smaller than the WF of the original wave packet since it is related to the probability of finding the electron scattered by a single phonon mode. The lifetime of the scattering electron, approximated with an exponential decrease of the unperturbed WF, is in fact due to the sum over all possible phonon out-scattering events.

A. Free propagation with phonon interaction

This is the simplest of the three considered cases, where only the quantum dynamics of the phonon scattering is studied without other complications due to electric fields or internal potential structures. The electron-phonon interaction is switched on at $t=2$ ps after the initial conditions.

The results are shown in Fig.1. The electron system is “observed” at the initial time $t = 0$ and at 0.5 and 1ps. The unperturbed WF of the scattering electron and the second-order correction (scattered electron)are shown together in separate arbitrary units, as discussed above.

It can be seen that the unperturbed electron moves towards the right with positive k , while the scattered electron moves towards the left with the negative k given by momentum conservation. As time increases the WF contour of the original electron elongates and it is slightly tilted. In order to understand this effect we note that each point of the WF for a free particle follows a classical trajectory [10], so that the higher-momentum components move faster than the lower-momentum components. In the Schrödinger wave-function description this corresponds to the well known wave-packet broadening with time; in the (q, p) Wigner representation the effect is described in more details. Furthermore, the height of the WF for the scattering electron is lowered by both the broadening of the electron wave packet and by its lifetime Γ^{-1} . The quantum continuum dynamics of the emission process is apparent from the elongated shape of the scattered WF. In contrast, the semiclassical approach would select a given final state in the phase-space domain where the WF is different from zero.

B. Propagation in presence of an electric field with phonon interaction

As a further example the propagation of an electron wave packet through a region of constant electric field has been examined. An electric field of strength $E = 5\text{kV/cm}$ extending over a length 2000\AA has been considered. The natural broadening of the electron

wave packet is amplified while the electron crosses the electric-field region. Fig. 2 shows the evolution of the unperturbed WF projected onto the plane (z, k_z) . A deformation of the form of the WF is observed while the wave packet crosses the field area (from -1000\AA to 1000\AA), due to the fact that, as time increases, the front of the WF experiences the field acceleration before the rear part. As the electron leaves the electric-field region a more elongated shape is observed due to the increased values of the momentum (and therefore velocity) components

Phonon scattering is switched on at $t = 0.2ps$ and the second-order perturbative correction to the WF due to the scattering process is evaluated at three successive times, as shown in Fig. 3 for the case $E = 0.5kV/cm$ between -1000\AA and -1000\AA . Again the scattered-electron WF is plotted together with the scattering-electron WF after a suitable rescaling and it is concentrated in k-space around the k value of the classical momentum conservation. It is observed at increasing times that the scattered electron is absent at the larger values of z reached by the scattering electron. In other words the scattering is no more effective after the electron has completely crossed the field area. This is so because the increased energy of the electron is no more compatible with energy and momentum conservation in an emission process of the mode (q, ω_q) . This is a manifestation of the intra-collision field effect and, for this reason, we have chosen a lower field value for the data in Fig. 3 ($E = 0.5kV/cm$), where some emission is still observed in the electric field region, while this is completely absent for the case $E = 5kV/cm$ as in Fig. 2.

C. Propagation through a double barrier with phonon interaction

A symmetrical double-barrier potential profile has been considered of height 0.2 eV, with barrier widths of 20\AA and well width of 100\AA .

The WF associated to the unperturbed motion of the electron wave packet is shown in Fig. 4. Due to the strong resonant condition of the electron wave packet, at 1 ps the WF exhibits a structure related to a large correlation effect in the phase space around

$z = 0$ (where the potential structure is located). At 1.5 ps the reflected and transmitted components of the electron wave packet have already emerged. The correlation effect can still be seen around $z = 0$ due to the coherence between the transmitted and the reflected part of the electron wave function.

Fig. 5 shows the scattered-electron WF at 1ps and 1.5ps. The interaction has been switched on at 0.5ps when the incoming electron approaches the double-barrier structure. At the shortest observation time a strong component in the perturbative correction appears in the phase space associated to the part of the electron wave packet scattered by the phonon before hitting the double barrier (let us call 'a' this type of event). As mentioned above, in our numerical case the final momentum ($k = -2.e8m^{-1}$) is almost reversed with respect to the value before scattering. At $t = 1.5ps$ other structures appear in the perturbative correction associated to positive z values corresponding to the electron scattered after transmission. The components associated to the negative p value represent the electron back-scattered after passing the potential profile (type 'b' event), while the components associated to the positive p are related to the electron that suffered the same back-scattering some time before, and has then been reflected towards the right by the double barrier (type 'c' event). The structure around vanishing p values at positive positions is due to the correlation between the two structures just described (i.e., between type 'b' and 'c' events). The structure around vanishing p values at negative positions is due to the correlation between the two structures indicated as type 'a' and type 'c'. Finally, also the WF due to the correlation between events of type 'a' and type 'b' can be seen in the figure at negative p and negative positions close to zero.

V. CONCLUSIONS

A theoretical approach to quantum transport based on the WF formalism has been used to study the quantum propagation of an electron wave packet in presence of a single phonon scattering event, taking into account the full continuum quantum dynamics of the interaction

in time. Three cases of increasing complexity have been examined, i.e., a) the effect of the quantum collision over a free propagation in space, where the collision duration allows for a distributions of final electron positions, b) the production of intra-collision field effect when the phonon interaction takes place while an electron wave packet propagates through a finite region of constant electric field, and finally c) the complex quantum-dynamical interference between potential profile and scattering when a wave packet propagates across a double-barrier structure in resonace conditions.

The analysis of quantum phonon scattering based on the theoretical approach presented in this paper is in progress: the application to the case of electrons in open systems is being analysed. In this case an incoming flux of particles from given boundaries of a quantum device must be considered instead of a single wave packet.

VI. ACKNOWLEDGEMENTS

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VII. FIGURE CAPTIONS

Fig.1 : Unperturbed WF (scattering electron) and the second-order correction (scattered electron) in a 3D plot at different times for an electron which propagates without external fields from $t = 0$ and experiences a quantum phonon emission beginning at $t = 0.2ps$ after the initial condition (see text).

Fig. 2 : Unperturbed WF (scattering electron) and the second-order correction (scattered electron) in a 2D (z, k_z) plot at different times for an electron which crosses a region of constant field ($E = 5kV/cm$).

Fig. 3 : Unperturbed WF (scattering electron) and the second-order correction (scattered electron) in a 3D plot at different times for an electron which crosses a region of constant field ($E = 0.5kV/cm$) and experiences a quantum phonon emission beginning at $t = 0.2ps$ after the initial condition (see text).

Fig. 4 : Unperturbed WF (scattering electron) at different times for an electron wave packet crossing a double barrier in resonant conditions (see text).

Fig. 5 : Second-order correction to the WF (scattered electron) at different times for the

electron wave packet reported in Fig. 4 during a quantum phonon emission beginning at $t = 0.5ps$ after the initial condition (see text).

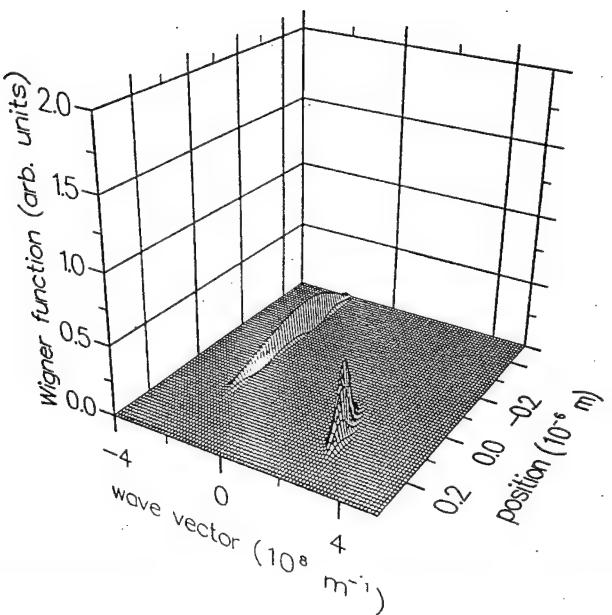
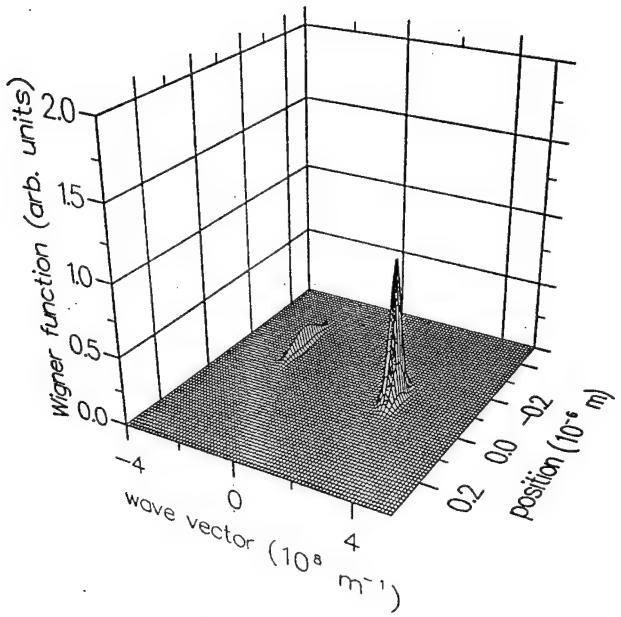
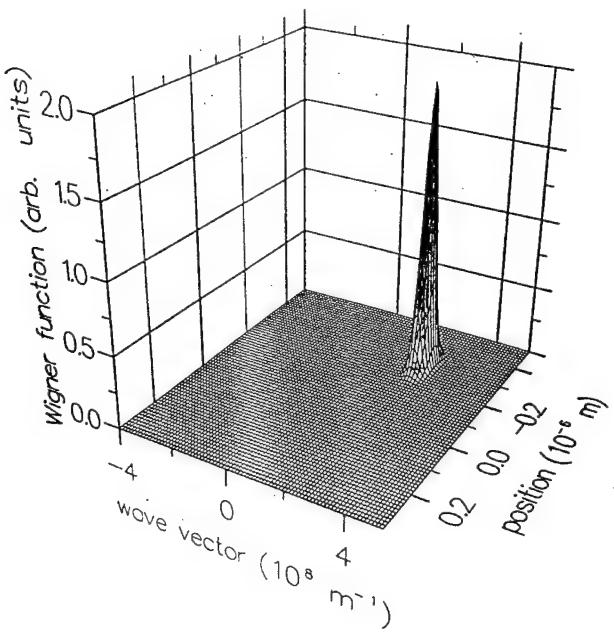


Fig. 1

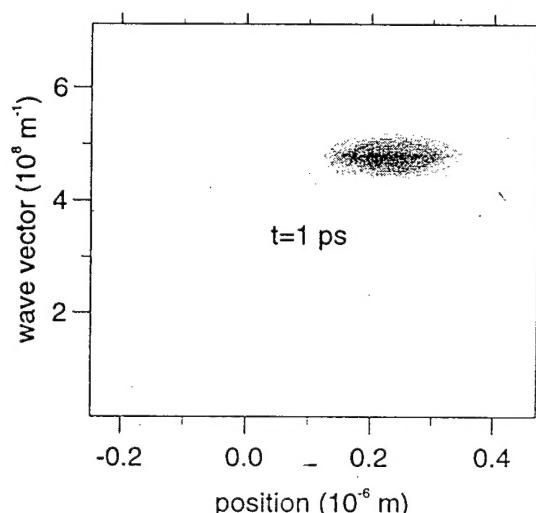
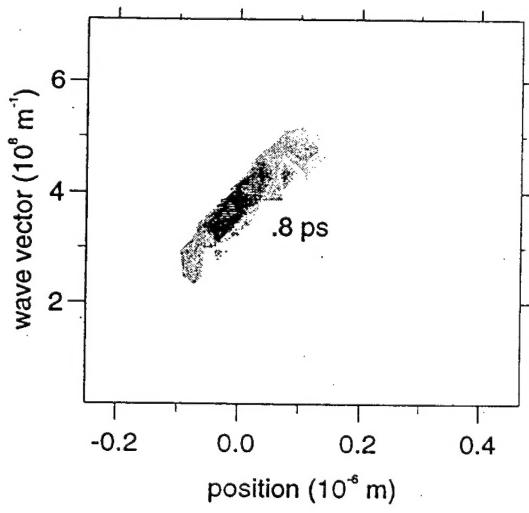
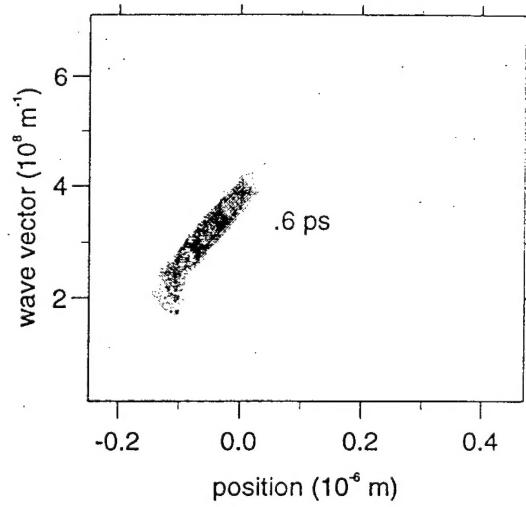
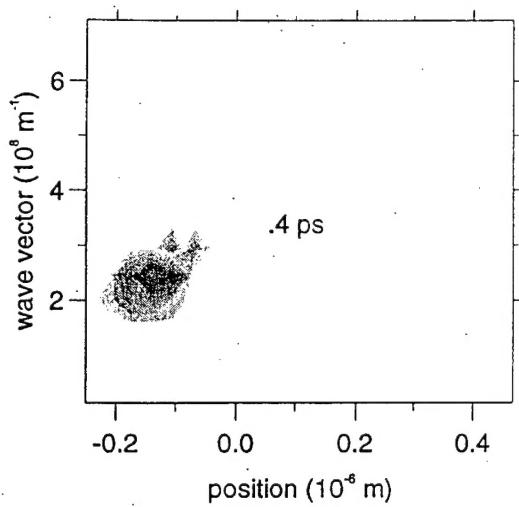


Fig 2

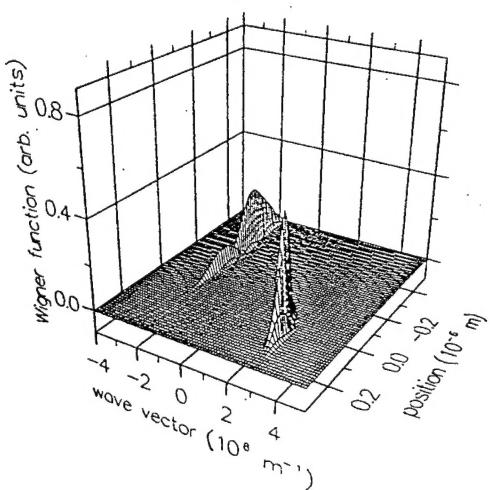
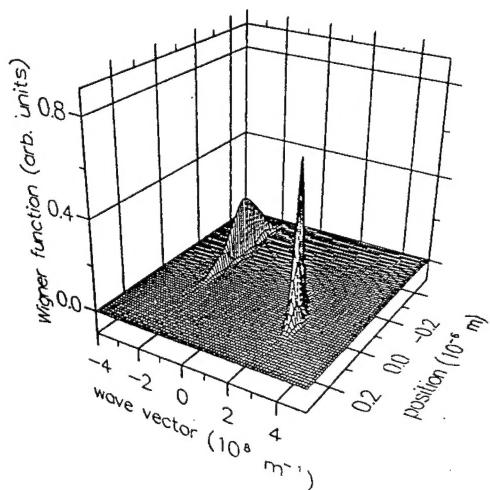
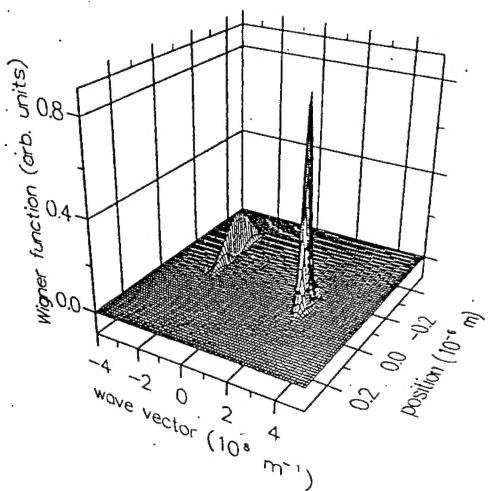


Fig. 3

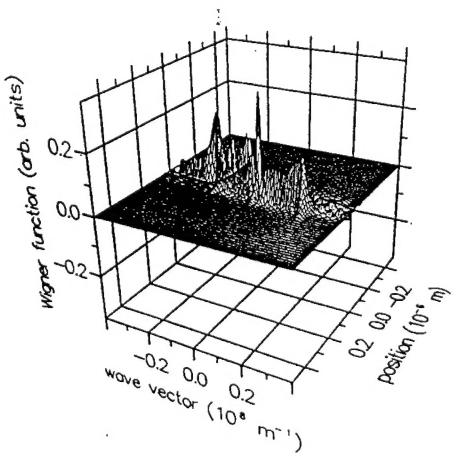
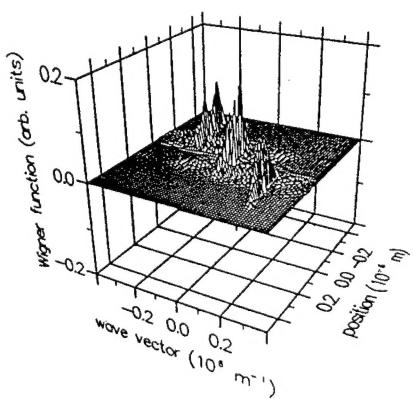
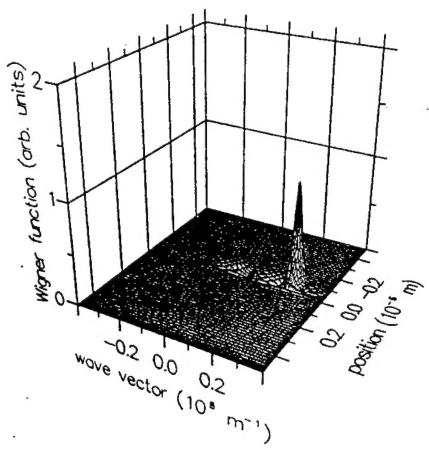
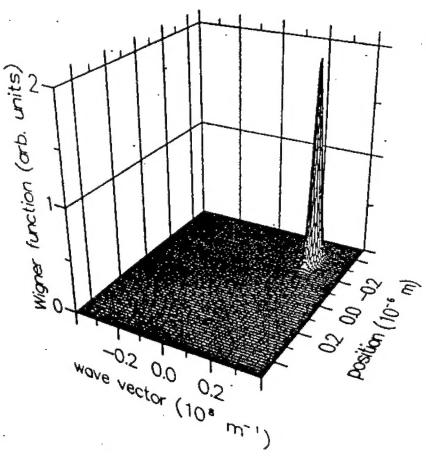


Fig 4

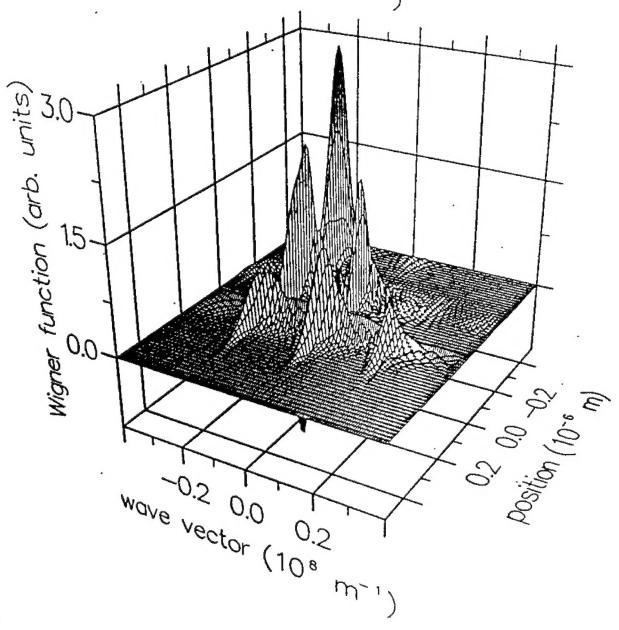
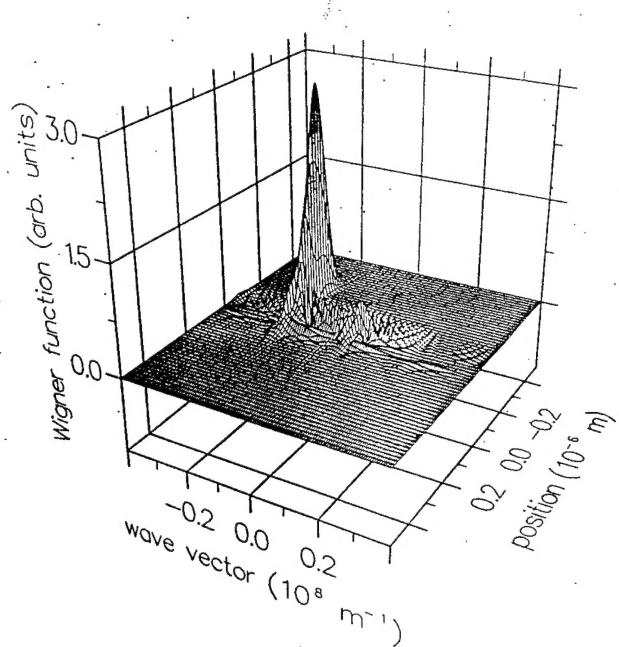


Fig. 5